Computation of Lattice Sums: Generalization of the Ewald Method

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The Ewald method was originally invented to compute the Madelung constant. In this paper we consider a lattice whose sites are associated with an arbitrary potential function. The "charge," or the scale factor for these potential functions, need not be the same at each site. We consider the evaluation of the resulting lattice sum at an arbitrary point, not necessarily at a lattice site. The method involves two generalizations over previous work: (1) the displacement of the origin off a lattice site and (2) the handling of arbitrary periodic charge distributions by decomposing such distributions into simpler ones involving only $+q$ and $-q$. The method should prove particularly useful for evaluating the expansion coefficients of the crystalline potential when this potential is expanded in the usual spherical harmonic series.

The problem of summing slowly converging series is an old one. One physical context in which the problem has been widely studied is the calculation of the potential due to an ionic crystal lattice. The methods of Madelung[1] and Evjen[2] depend on collecting ions into neutral groups. The convergence obtained in this way, however, is conditional: that is, the result depends on the way in which the neutral groups are chosen. Ewald's[3] method, which hinges on doing part of the summation in reciprocal space, gives rapid convergence and the limit is unique. Subsequent discussions[4-10] of this topic have been extensions and generalizations of these methods. This work too is an extension of the Ewald technique. In particular it is a generalization of the approach taken by Nijboer and DeWette.[9]

For purposes of orientation, we summarize the basic philosophy of the Ewald method. Suppose we have a function $\varphi(r)$ such that the series

$$S = \sum_{n=1}^{\infty} \varphi(\mathbf{r}_n) \tag{1}$$

is slowly converging. The symbol $\sum_n$ is to be understood as a shorthand for $\sum_{n_1} \sum_{n_2} \sum_{n_3}$. It represents independent summation on all three components of the vector $\mathbf{r}$. We now construct some function $g(\mathbf{r})$, which falls off rapidly with r, and its partner

$$f(\mathbf{r}) = 1 - g(\mathbf{r}), \tag{2}$$

which rapidly approaches unity as $\mathbf{r}$ increases. We now write

$$S = \sum_n \varphi(\mathbf{r}_n) g(\mathbf{r}_n) + \sum_n \varphi(\mathbf{r}_n) f(\mathbf{r}_n). \tag{3}$$

The first sum converges rapidly, because of g. The second sum converges like φ, i.e., slowly. Its Fourier transform, however, will converge rapidly. In fact the more slowly this sum converges the more rapidly will its transform converge. To complete the argument we need Parseval's theorem:

If

$$\Phi(\mathbf{h}) = \int \exp(i2\pi\mathbf{h}\cdot\mathbf{r})\varphi(\mathbf{r})\, d\mathbf{r} \tag{4a}$$

and

$$F(\mathbf{h}) = \int \exp(i2\pi\mathbf{h}\cdot\mathbf{r}) f(\mathbf{r})\, d\mathbf{r} \tag{4b}$$

then

$$\int \Phi(\mathbf{h}) F^*(\mathbf{h})\, d\mathbf{h} = \int \varphi(\mathbf{r}) f^*(\mathbf{r})\, d\mathbf{r} \tag{4c}$$

where the symbol * denotes "complex conjugate." The formal passage from sums to integrals can be accomplished by means of Dirac delta functions $\delta(\mathbf{r} - \mathbf{r}_n)$, as we shall see below. Thus Parseval's theorem guarantees that the summation in transform space yields the same result as the summation in the original coordinate space.

We now apply this scheme to the calculation of the potential due to an ionic lattice. To begin with, we consider what we shall call a "primitive" lattice. Such a lattice is generated from primitive translations $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$ in such fashion that

$$\mathbf{r}_n = \sum_{i=1}^{3} n_i \mathbf{c}_i, \tag{5}$$

with n_1, n_2, n_3 taking on independently all integer values from $-\infty$ to ∞; and in addition there is associated with each lattice point $\mathbf{r}_n$ a charge

$$q_n = q_0(-1)^{n_1+n_2+n_3} \tag{6}$$

where q_0 is some constant. A typical primitive lattice is NaCl, in contrast, for instance, to CaF_2, which does not obey (6).

We define reciprocal vectors $\mathbf{h}_i$ by the usual relation

$$\mathbf{h}_i \cdot \mathbf{c}_j = \delta_{ij} \tag{7}$$

and the reciprocal lattice as the aggregate of points

$$\mathbf{h}_n = \sum n_i \mathbf{h}_i \tag{8}$$

where the n's again run from $-\infty$ to ∞. It is trivial to show that if these two lattices are represented respectively as $\sum_n \delta(\mathbf{r} - \mathbf{r}_n)$ and $\sum_n \delta(\mathbf{h} - \mathbf{h}_n)$, then the reciprocal lattice is simply the Fourier transform of the coordinate lattice, the Fourier transform being understood as in (4a) and (4b). If we define the special reciprocal lattice vector

$$\mathbf{k} = \tfrac{1}{2}(\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3), \tag{9}$$

then (6) can be rewritten

$$q_n = q_0 \exp\ (i2\pi\mathbf{k}\cdot\mathbf{r}_n). \tag{10}$$

In addition to q_n, we associate with each lattice point a function $\varphi(\mathbf{r})$. For the present we place no restriction on $\varphi(\mathbf{r})$, except that it possess a Fourier transform. Of course there would be no practical motivation for the calculation unless $\varphi(\mathbf{r})$ fell off slowly with $\mathbf{r}$. We wish to sum the contribution of all the φ's at some arbitrary point $\mathbf{R}$:

$$S = \sum_n \varphi(\mathbf{r}_n - \mathbf{R}) \exp\ (i2\pi\mathbf{k}\cdot\mathbf{r}_n). \tag{11}$$

To change the sum into an integral, as required for the eventual application of (4c), we define

$$w(\mathbf{r}) = \exp\ (i2\pi\mathbf{k}\cdot\mathbf{r}) \sum_n \delta(\mathbf{r} - \mathbf{r}_n), \tag{12}$$

so that

$$S = \int w(\mathbf{r})\varphi(\mathbf{r} - \mathbf{R})d\mathbf{r}. \tag{13}$$

In exact analogy to (2) and (3) we can break S into two parts:

$$S = \int w(\mathbf{r})\varphi(\mathbf{r} - \mathbf{R})g(\mathbf{r} - \mathbf{R})d\mathbf{r} + \int w(\mathbf{r})\varphi(\mathbf{r} - \mathbf{R})f(\mathbf{r} - \mathbf{R})d\mathbf{r}. \tag{14}$$

The first integral in (14) corresponds to the first sum in (3):

$$\sum_n \varphi(\mathbf{r}_n - \mathbf{R}) g(\mathbf{r}_n - \mathbf{R}) (-1)^{n_1+n_2+n_3}. \tag{15}$$

The second integral we wish to evaluate in the conjugate domain. For brevity we define

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) f(\mathbf{r}) \tag{16}$$

$$\Psi(\mathbf{h}) = \int_{-\infty}^{\infty} \exp(i2\pi\mathbf{h}\cdot\mathbf{r})\, \psi(\mathbf{r})\, d\mathbf{r}. \tag{17}$$

Then the Fourier transform of $\varphi(\mathbf{r} - \mathbf{R}) f(\mathbf{r} - \mathbf{R})$ is given by

$$\int_{-\infty}^{\infty} \exp(i2\pi\mathbf{h}\cdot\mathbf{r})\, \psi(\mathbf{r} - \mathbf{R})\, d\mathbf{r} = \exp i2\pi\mathbf{h}\cdot\mathbf{R}\, \Psi(\mathbf{h}). \tag{18}$$

The transform of $w(r)$ is easily evaluated (see Ref. 9) and is given by

$$\int_{-\infty}^{\infty} \exp(i2\pi\mathbf{h}\cdot\mathbf{r})\, w(\mathbf{r})\, d\mathbf{r} = \frac{1}{v_c} \sum_n \delta(\mathbf{h} + \mathbf{k} - \mathbf{h}_n), \tag{19}$$

where v_c equals $\mathbf{c}_1\cdot\mathbf{c}_2 \times \mathbf{c}_3$, or the volume of the coordinate unit cell. By Parseval's theorem [(4a), (4b), (4c)], the second integral of (14) now becomes

$$\frac{1}{v_c} \sum_n \exp[i2\pi(\mathbf{h}_n - \mathbf{k})\cdot\mathbf{R}]\, \Psi(\mathbf{h}_n - \mathbf{k}). \tag{20}$$

This completes the essential derivation, since S is now expressed in terms of the two sums (15) and (20), both of which converge rapidly.

We consider some special cases. If $\mathbf{R} = 0$ — that is, if we are sitting at a lattice point — we presumably will want to exclude the contribution of that point itself. If $\varphi(0)$ is finite, the contribution can be subtracted outright. If $\varphi(0)$ diverges, as is usually the case, one must be clever about picking the functions g and f so that $\psi(0) = f(0)\varphi(0)$ does not diverge. One then simply omits from the sum (15) the term for $n = 0$, and subtracts from the sum (20) the quantity $\psi(0)$. Note that one subtracts $\psi(0)$, not $\Psi(0)$. The Ewald calculation is obtained in this way, if one takes

$$\varphi(\mathbf{r}) = |\mathbf{r}|^{-1} \tag{21a}$$

$$g(\mathbf{r}) = \mathrm{Erfc}\ (|\mathbf{r}|) \tag{21b}$$

$$f(\mathbf{r}) = \mathrm{Erf}\ (|\mathbf{r}|). \tag{21c}$$

We note that if φ is real (for example, any central potential) and if we pick g real, then ψ will be real also. The function w is both real and

symmetric because of our particular definition of the reciprocal vector $\mathbf{k}$. It follows that the sum S as defined in (14) is real. But if we look at the partial sum (20), this reality is not at first sight apparent, since the $\mathbf{R}$ can be chosen arbitrarily. But ψ real implies that Ψ is Hermitian: $\Psi(-\mathbf{h}_n + \mathbf{k}) = \Psi^*(\mathbf{h}_n - \mathbf{k})$, and clearly $\exp[i2\pi(\mathbf{h}_n - \mathbf{k})\cdot\mathbf{R}]$ is Hermitian. Again, because of the peculiar choice of $\mathbf{k}$, the arguments $\pm(\mathbf{h}_n - \mathbf{k})$ are bound to occur in pairs. Since the sum of a function and its complex conjugate is real, the sum (20) is always real, which we may emphasize by rewriting it:

$$\frac{2}{v_c}\,\mathrm{Re}\sum_n^{+}\exp[i2\pi(\mathbf{h}_n - \mathbf{k})\cdot\mathbf{R}]\,\Psi(\mathbf{h}_n - \mathbf{k}). \tag{22}$$

Here $\sum^{+}$ means that we sum only over half the space. This can be accomplished by summing n_3, for instance, from 1 to ∞ instead of from $-\infty$ to ∞.

If $\psi(\mathbf{r})$ is symmetric, $\Psi(\mathbf{h})$ will be real, and in the sum (22) we will obtain only cosine terms. Conversely, if $\psi(\mathbf{r})$ is antisymmetric, the reciprocal sum will contain only sine terms. Again this is independent of the choice of $\mathbf{R}$.

We now also see clearly why the Ewald method "works." The convergence difficulties with the series S of (1) concern its asymptotic behavior. But this behavior is related to the behavior at the origin of the series in reciprocal space.[12] By means of the vector $\mathbf{k}$, we guarantee avoidance of the origin in reciprocal space, regardless of any other conditions in the problem.

The sums that most frequently occur in practice are related to the expansion of the crystalline potential in spherical harmonics:

$$V(x) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_{lm}\,|\,x\,|^{l}\,Y_{l,-m}\,(\theta_x\,,\,\varphi_x) \tag{23}$$

$$C_{lm} = \frac{4\pi}{2l+1}\sum_n q_n\,|\,\mathbf{r}_n\,|^{-l-1}\,Y_{l,m}\,(\theta_{\mathbf{r}_n}\,,\,\varphi_{\mathbf{r}_n}) \tag{24}$$

$$Y_{l,m}\,(\theta,\varphi) = \left[\frac{2l+1}{4\pi}\cdot\frac{(l-|\,m\,|)!}{(l+|\,m\,|)!}\right]^{\frac{1}{2}} e^{im\varphi}\,P_{lm}(\theta). \tag{25}$$

The notation is well known and conventional. Our definition of the spherical harmonics Y_{lm} implies ${Y_{lm}}^* = Y_{l-m}$. Also $Y_{lm}(\pi-\theta,\pi+\varphi) = (-1)^l Y_{lm}(\theta,\varphi)$. The evaluation of the crystal sums C_{lm} has been discussed by Nijboer and DeWette.[9] In our notation, $\varphi(\mathbf{r})$ here corresponds to $r^{-l-1}Y_{lm}(\theta,\varphi)$. Nijboer and DeWette's choice of g is the incomplete gamma function[11]

$$g(\mathbf{r}) = \Gamma(n + l,\pi r^2)/\Gamma(n + l) \tag{26a}$$

$$f(\mathbf{r}) = 1 - g(\mathbf{r}) = \gamma(n + l,\pi r^2)/\Gamma(n + l). \tag{26b}$$

They solve the problem subject to the restrictions that (a) the potential is expanded about a lattice point, i.e., $\mathbf{R} = 0$, and (b) the lattice is primitive, in the sense of (5), (6) and (10). Our discussion has made it obvious how to remove the first restriction. Generalizing their result, via (20),

$$\begin{aligned} C_{lm}(\mathbf{r} - \mathbf{R}) = {} & \frac{4\pi}{2l + 1} \cdot \frac{1}{\Gamma(l + \frac{1}{2})} \\ & \cdot [\sum_n | \mathbf{r}_n - \mathbf{R} |^{-l-1} \Gamma(l + \tfrac{1}{2},\pi | \mathbf{r}_n - \mathbf{R} |^2) Y_{lm}(\theta_{\mathbf{r}_n - \mathbf{R}} , \varphi_{\mathbf{r}_n - \mathbf{R}}) \\ & \cdot \exp (i2\pi \mathbf{k} \cdot \mathbf{r}_n) \\ & + i^l \pi^{l-\frac{1}{2}} v_c^{-1} \sum_n \exp (i2\pi (\mathbf{h}_n - \mathbf{k}) \cdot \mathbf{R}) | \mathbf{h}_n - \mathbf{k} |^{l-2} \\ & \cdot \Gamma(1,\pi | \mathbf{h}_n - \mathbf{k} |^2) \times Y_{lm}(\theta_{\mathbf{h}_n - \mathbf{k}} , \varphi_{\mathbf{h}_n - \mathbf{k}})]. \end{aligned} \tag{27}$$

The next generalization of the procedure lies in its application to nonprimitive lattices. Such application will clearly be possible if an arbitrary lattice can be decomposed into a sum of component primitive lattices. We illustrate what we mean by a one-dimensional example. Consider a one-dimensional lattice with charges distributed as follows:

$$L = 2\ 1\ 0\ -3\ 2\ 1\ 0\ -3\ 2\ 1\ 0\ -3\ \cdots .$$

Thus we have $q_1 = 2$, $q_2 = 1$, $q_3 = 0$, $q_4 = -3$. If the distance between successive q's is 1 distance unit, then the basic periodicity is 4. We note that $\sum q = 0$, since we must have a neutral lattice, and that zero is itself an allowable q value. Now consider the following sequences of numbers of periodicity 4:

$$L_1 = \tfrac{1}{2}\ -\tfrac{1}{2}\ \tfrac{1}{2}\ -\tfrac{1}{2}\ \cdots$$

$$L_2 = \frac{1}{\sqrt{2}}\ 0\ -\frac{1}{\sqrt{2}}\ 0\ \cdots$$

$$L_3 = 0\ \frac{1}{\sqrt{2}}\ 0\ -\frac{1}{\sqrt{2}}\ \cdots .$$

We can represent L as the sum $L = 2L_1 + \sqrt{2}\, L_2 + 2\sqrt{2}\, L_3$. We

note that L_1, L_2, L_3 are all primitive since they fulfill both (5) and the two equivalent equations (6) and (10). In terms of (5), for L_1, $|\mathbf{c}| = 1$; for L_2 and L_3, $|\mathbf{c}| = 2$, but their origin of coordinates is shifted by one unit.

We can define a dot product for the L's in the following sense. Suppose we have $L_A = \sum_i q_i^{(A)} \delta(\mathbf{r} - \mathbf{r}_i)$ and $L_B = \sum_i q_i^{(B)} \delta(\mathbf{r} - \mathbf{r}_i)$. Then $L_A \cdot L_B = \sum_i q_i^{(A)} q_i^{(B)}$, where the sum runs over a unit cell. We note that, in our example, the components L_i are orthonormal, and that the projection of L on each L_i can be found by taking the dot product.

We also observe that we have three components, which is just enough to account for 4 numbers which are subject to the one constraint $\sum q_i = 0$. Our three components L_i "span the space" of L, and it is clear in general that if L consists of a periodic sequence of P numbers whose sum is zero, we shall need $(P - 1)$ primitive components.

The question is: Is it possible to decompose an arbitrary periodic sequence L into orthonormal primitive components? Can one devise an algorithm for finding these components? Can one do this in three dimensions? In considering these questions, we have collaborated with Dr. R. L. Graham, and we are particularly indebted to him for pointing out the great simplification that results if one confines oneself to sequences of periodicity 2^n in each dimension.

Consider a linear sequence L of periodicity 2^n. If $\mathbf{c}$ is the primitive translation of L, we define $\mathbf{a} = \mathbf{c}/2^n$. The basic vectors for generating primitive component lattices are $\mathbf{b}^{(1)} = \mathbf{a}$, $\mathbf{b}^{(2)} = 2\mathbf{b}^{(1)}$, $\cdots$ $\mathbf{b}^{(n)} = 2\mathbf{b}^{(n-1)}$. Each $\mathbf{b}^{(i)}$ for $i > 1$, will generate a *set* of primitive lattices differing only in their choice of origin. There will evidently be n such sets of components. Primitive component lattices containing 2^m nonzero entries per unit cell will have a basis vector of length $|\mathbf{c}|/2^{n-m}$ and will have 2^{n-m} possible shifts of origin. We note that $\sum_{m=1}^{n} 2^{n-m} = 2^n - 1$, which is the correct total number of components. The number of primitive components of the same periodicity but with shifted origins doubles every time the length of the generating basic vector $\mathbf{b}_i$ doubles, and of course the number of nonzero entries per unit cell halves at the same time. The set of origin positions $\{\mathbf{R}_i\}$ associated with $\mathbf{b}_i$ is clearly the set of all translations $\mathbf{R}$ such that $\mathbf{R}_i - \mathbf{R}_j \neq \mathbf{b}_i$. This includes the set $\{\mathbf{R}_{i-1}\}$ plus a new set formed by adding $\mathbf{b}_{i-1}$ to all $\mathbf{R}$ in $\{\mathbf{R}_{i-1}\}$.

All the primitive component lattices are orthogonal to each other, in the sense that $L_i \cdot L_j = \delta_{ij}$. Within each "phase-shifted" set, each

component has numbers in locations where all the other components have zero, so that the members of such a set are obviously orthogonal. Now consider two sequences L_i and L_{i-1} belonging to sets generated by $\mathbf{b}_i$ and $\mathbf{b}_{i-1}$. Either L_{i-1} will have numbers only where L_i has zero. Otherwise, each alternate number in L_{i-1} will have zero as a partner in L_i; the remaining numbers in L_{i-1} all have the same sign, but their nonzero partners in L_i have alternating signs. Hence once again the dot product is zero. The same argument applies clearly not only to members of contiguous sets L_i and L_{i-1}, but to members of any two sets, L_i and L_j, $i \neq j$. To produce not merely orthogonality, but orthonormality over the unit cell, the normalization factor, or q_0 in (6) and (10), must clearly be $2^{-m/2}$ for a component with 2^m nonzero entries.

In the example we have given, $n = 2$, and all the above arguments can be seen to be rather trivially verified.

Extension of the preceding to two dimensions is straightforward. We consider a two-dimensional array, doubly periodic with periodicity $2^n \times 2^n$. The primitive translations $\mathbf{c}_1$ and $\mathbf{c}_2$ carry any q into the corresponding q in another cell. Within each cell, the different q's are separated by multiples of $\mathbf{c}_1/2^n$ and $\mathbf{c}_2/2^n$, and we shall call these vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. As before, we define a set of components of equal periodicity by defining the basic vectors which will generate the primitive lattice. The translations by which components within a set differ we denote by R. The algorithm for producing a complete orthonormal set of components is simple:

$$\mathbf{b}_1^{(1)} = \mathbf{a}_1 \tag{28a}$$

$$\mathbf{b}_2^{(1)} = \mathbf{a}_2 \tag{28b}$$

$$\mathbf{b}_1^{(2)} = \mathbf{a}_1 + \mathbf{a}_2 \tag{28c}$$

$$\mathbf{b}_2^{(2)} = \mathbf{a}_1 - \mathbf{a}_2 \tag{28d}$$

$$\mathbf{b}_1^{(n+2)} = 2\mathbf{b}_1^{(n)} \tag{28e}$$

$$\mathbf{b}_2^{(n+2)} = 2\mathbf{b}^{(n)} \tag{28f}$$

$$q^{(1)} = 2^{-n} \tag{29a}$$

$$q^{(n)} = q^{(n-1)}\sqrt{2} \tag{29b}$$

$$\{\mathbf{R}^{(1)}\} = 0 \tag{30a}$$

$$\{\mathbf{R}^{(n+1)}\} = \{\mathbf{R}^{(n)}\} + \{\mathbf{R}^{(n)} + \mathbf{b}_1^{(n)}\}. \tag{30b}$$

The set labels appear as superscripts in (28–30). The vectors $\mathbf{b}$ are the basis of a primitive lattice, and $\{\mathbf{R}\}$ indicates the set of all translations $\mathbf{R}$ which relate primitive lattices having the same basis. Equation (30b) says that the translations for set n include all the translations for set $n-1$, plus all translations formed by adding any *one* of the vectors $\mathbf{b}^{n-1}$ to all the $\mathbf{R}$'s of set $n-1$. Again all components are orthonormal over the unit cell, so that the decomposition of any $2^n \times 2^n$ dimensional cell can simply be found by taking dot products. Normalization is insured by our definition of q_n, and orthogonality becomes clear from the same type of reasoning as in the linear case, which we shall not repeat here.

In three dimensions, we consider an array triply periodic with periodicity $2^n \times 2^n \times 2^n$. We define $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$, and $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ in analogy with the two-dimensional case. We present the basic vectors for the primitive lattices, plus the associated translations:

$$\mathbf{b}_1^{(1)} = \mathbf{a}_3 \tag{31a}$$

$$\mathbf{b}_2^{(1)} = \mathbf{a}_2 \tag{31b}$$

$$\mathbf{b}_3^{(1)} = \mathbf{a}_2 + \mathbf{a}_1 \tag{31c}$$

$$\mathbf{b}_1^{(2)} = \mathbf{a}_3 + \mathbf{a}_2 \tag{31d}$$

$$\mathbf{b}_2^{(2)} = -\mathbf{a}_3 + \mathbf{a}_2 \tag{31e}$$

$$\mathbf{b}_3^{(2)} = \mathbf{a}_1 \tag{31f}$$

$$\mathbf{b}_1^{(3)} = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 \tag{31g}$$

$$\mathbf{b}_2^{(3)} = \mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 \tag{31h}$$

$$\mathbf{b}_3^{(3)} = \mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 \tag{31i}$$

$$\mathbf{b}_1^{(n+3)} = 2\mathbf{b}_1^{(n)} \tag{31j}$$

$$\mathbf{b}_2^{(n+3)} = 2\mathbf{b}_2^{(n)} \tag{31k}$$

$$\mathbf{b}_3^{(n+3)} = 2\mathbf{b}_3^{(n)} \tag{31l}$$

$$q^{(1)} = 2^{-3n/2} \tag{32a}$$

$$q^{(n+1)} = q^n \sqrt{2} \tag{32b}$$

$$\{\mathbf{R}^{(1)}\} = 0 \tag{33a}$$

$$\{\mathbf{R}^{(n+1)}\} = \{\mathbf{R}^n\} + \{\mathbf{R}^{(n)} + \mathbf{b}_1^{(n)}\}. \tag{33b}$$

The choice of b's is not unique, and we have given a set that seems to bear a maximum analogy to the two-dimensional case.

Many lattices can be represented as $2^n \times 2^n \times 2^n$ dimensional arrays. We note that the primitive translations $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$ need not be orthogonal. Even if a lattice does not lend itself to such a representation, by choosing a fine enough grid (with a correspondingly large number of zero charges), one can approximate any lattice to any desired degree of accuracy.*

We now return to the problem of the lattice sum. We will obtain a sum of the type (20), or more specifically of the type (27a), for each primitive component. For a particular set of components which are translated from each other by $\{\mathbf{R}_n\}$, it clearly makes no difference whether we sum the contribution of each component at the origin or the contribution of any one component at the points given by $\{\mathbf{R}_n\}$. (The difference between shifting the function and shifting the coordinate system is merely a conceptual one.) Hence the shift vectors $\mathbf{R}_n$ correspond to the position vectors $\mathbf{R}$ in expressions (20) and (27a).

In the present approach, we have completely split the geometrical character of the lattice from the charges assigned to each lattice point. This suggests the possibility of computing the lattice sums arising from all the primitive components of commonly occurring grids, once and for all. The problem of computing a particular lattice sum would then involve only the decomposition of the given lattice into primitive component lattices, whose contribution to the sum would already be known. Work along this line is in progress.

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* The restriction of $2^n \times 2^n \times 2^n$ dimensional arrays is in fact too rigid. It is possible to formulate necessary and sufficient conditions for the decomposability of an arbitrary grid; to prove the existence of a complete set of orthogonal primitive lattices when the decomposition is possible; and to provide simple algorithms for constructing these lattices. These more general results have been derived by Dr. R. L. Graham, and we are grateful for access to them prior to publication.

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